

Double Well Potential Function and Its Optimization in the n -dimensional Real Space – Part II

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Abstract

In contrast to taking the dual approach for finding a global minimum solution of a double well potential function, in Part II of the paper, we characterize a local minimizer, local maximizer, and global minimizer directly from the primal side. It is proven that, for a “nonsingular” double well function, there exists at most one local, but non-global, minimizer and at most one local maximizer. Moreover, when it exists, the local maximizer is “surrounded” by local minimizers in the sense that the norm of the local maximizer is strictly less than that of any local minimizer. We also establish some necessary and sufficient optimality conditions for the global minimizer, local non-global minimizer and local maximizer by studying a convex secular function over specific intervals. These conditions lead to three algorithms for identifying different types of critical points of a given double well function.

Keywords: Double well potential, Local minimizer, Local maximizer, Global minimum.

1 Introduction

In Part I, the double well potential problem (DWP) is defined by

$$\min_{x \in R^n} \left\{ \Pi(x) = \frac{1}{2} \left(\frac{1}{2} \|Bx - c\|^2 - d \right)^2 + \frac{1}{2} x^T A x - f^T x \right\}, \quad (1)$$

where A is an $n \times n$ real symmetric matrix, $B \neq 0$ is an $m \times n$ real matrix, $c \in R^m$, $d \in R$ and $f \in R^n$. By introducing a continuous variable transformation $\xi = \frac{1}{2}\|Bx - c\|^2 - d$, the double well potential problem (DWP) can be transformed into the following equivalent quadratic program over one nonhomogeneous quadratic constraint (QP1QC):

$$\min \quad \Pi(x, \xi) = \frac{1}{2}\xi^2 + \frac{1}{2}x^T Ax - f^T x \quad (2)$$

$$\text{s.t.} \quad \xi = \frac{1}{2}\|Bx - c\|^2 - d, \quad x \in R^n. \quad (3)$$

The dual problem of (QP1QC) and the dual of the dual were studied in Part 1 (Theorem 1) in order to find a global minimum solution to problem (DWP).

For practical applications, knowing only the global minimum of a double well potential function may not be sufficient. For example, the double well potential model can be used to describe the ion-molecule reactions, where the intermediate molecule complexes must go across the energy barrier to cause reactions [2]. Researchers have to know the potential difference between the energy wells (caused by local minima) and energy barrier (caused by local maximum). The understanding of all types of critical points of a double well function is thus necessary.

Mathematically, we are motivated by the pioneering work of Martínez [8] which showed that a trust-region subproblem (TRS) [5] of the following form

$$\min \quad \frac{1}{2}x^T Ax - f^T x \quad (4)$$

$$\text{s.t.} \quad \|x\|^2 = \Delta, \quad x \in R^n \quad (5)$$

(with Δ being a positive scalar) has at most one local, but non-global, minimizer. Please notice that, on one hand, problem (QP1QC) can be regarded as an extension of problem (TRS) towards the nonhomogeneous and possibly singular case. On the other hand, the penalty version of the trust-region subproblem, namely,

$$\min_{x \in R^n} \frac{1}{2}x^T Ax - f^T x + \theta(\|x\|^2 - \Delta)^2$$

(with the penalty parameter θ being sufficiently large) is clearly a special case of the double well potential problem (DWP). Therefore, our approach to analyzing the local non-global minimizer of a double well potential problem extends the results of [8]. Moreover, when restricted to problem (TRS), our approach simplifies the proof provided in [8]. Although, in general, a double well potential problem may have infinitely many local, but non-global, minimizers (see Figure 1), we'll show that, after taking the space reduction technique developed in Section 2 of Part I, the reduced nonsingular problem has at most one local non-global minimizer and at most one local maximizer.

We remark that characterizing the local maximizer of the trust-region subproblem (4)-(5) can be reduced to the problem of finding a local minimizer of (4) with A being replaced by $-A$. However, due to the non-symmetric nature, it is no longer the case for the double well potential problem (1).

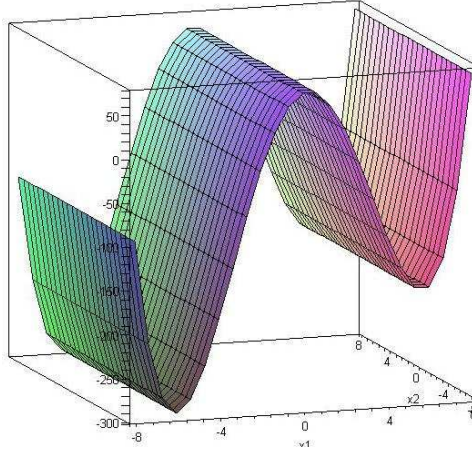


Figure 1: A double well potential problem having infinitely many local non-global minima.

Hence Martínez's approach may not be able to characterize the local maximizer for a general (DWP) problem.

In the rest of the paper, a characterization of the local, but non-global, minimizer of a double well function is provided in Section 2. Then, a characterization of the global minimizer of a double well function is given in Section 3, while the local maximizer is characterized in Section 4. Computational algorithms for each type of the optimizers of a double well potential function are proposed in Section 5 with some illustrative examples. Some concluding remarks are given in Section 6.

Here we define some notations to be used throughout the paper. Let S^n be the set of all n -dimensional symmetric real matrices, S_+^n be the set of all n -dimensional positive semi-definite matrices, and S_{++}^n be the set of all n -dimensional positive definite matrices. For any $P, Q \in S^n$, $P \succeq Q$ means that matrix $P - Q \in S_+^n$ and $P \succ Q$ means that matrix $P - Q \in S_{++}^n$. We sometimes write $Q \preceq P$ for $P \succeq Q$ and $Q \prec P$ for $P \succ Q$. The i th smallest eigenvalue of $P \in S^n$ is denoted by $\sigma_i(P)$ and the determinant of P by $\det(P)$. The n -dimensional identity matrix is denoted by I . For a vector $x \in R^n$, $x \geq 0$ ($x > 0$) means that each component of x is nonnegative (positive) and $\text{Diag}(x)$ is an n -dimensional diagonal matrix with diagonal components being x_1, \dots, x_n . Moreover, for a number $\beta \in R^n$, $\text{sign}(\beta) = \frac{\beta}{|\beta|}$ if $\beta \neq 0$, otherwise $\text{sign}(\beta) = 0$.

2 Characterization of local non-global minimizer

Following the space reduction technique developed in Part I, without loss of generality, we may assume that, in problem (BWP), $B^T B$ is positive definite such that, matrices A and $B^T B$ are simultaneously diagonalizable via congruence, i.e., there is a nonsingular matrix P such that $D \triangleq$

$P^T A P = \text{Diag}(\alpha_1, \dots, \alpha_n)$ with $\alpha_1 \leq \dots \leq \alpha_n$ and $P^T B^T B P = I$. It follows immediately that $(B^T B)^{-1} = P P^T$. Let

$$w = P^{-1}x - P^T B^T c,$$

then we have

$$\begin{aligned} \frac{1}{2}\|Bx - c\|^2 - d &= \frac{1}{2}\|B(Pw + P P^T B^T c) - c\|^2 - d \\ &= \frac{1}{2}w^T w + \frac{1}{2}c^T (I - B(B^T B)^{-1} B^T) c - d \end{aligned}$$

and

$$\frac{1}{2}x^T A x - f^T x = \frac{1}{2}w^T D w + c^T B P D w + \frac{1}{2}c^T B P D P^T B^T c - f^T P w - f^T P P^T B^T c.$$

For simplicity, we define $\nu = -\frac{1}{2}c^T (I - B(B^T B)^{-1} B^T) c + d$ and $\psi = P^T f - D P^T B^T c$. By dropping the constant terms, we can rewrite problem (DWP) defined in (1) as

$$\min \left\{ g(w) = \frac{1}{2} \left(\frac{1}{2}\|w\|^2 - \nu \right)^2 + \frac{1}{2}w^T D w - \psi^T w \right\}. \quad (6)$$

Recall that the canonical primal problem defined in (19) of Part I is to minimize

$$\frac{1}{2} \left(\frac{1}{2}\|w\|^2 - \varphi^T w - \nu \right)^2 + \frac{1}{2}w^T D w - \psi^T w. \quad (7)$$

The form in (6) is a further simplified version of form (7) by setting $\varphi = 0$. In this way, the third order term in problem (DWP) is eliminated and the complexity is decreased for analysis. It's interesting to note that, in the finite deformation theory, the diagonal matrix D represents the material constants, the first order coefficient vector ψ stands for the external forces, and the Cauchy-Green strain $\frac{1}{2}\|w\|^2 - \nu$ measures the square of local changes in distance due to deformation. As we shall observe below, the first order and the second order necessary conditions of (6) (see [9]) are highly related to the term of $(\frac{1}{2}\|w\|^2 - \nu)I + D$, which is the sum of the Cauchy-Green strain and the material constants. Our first result of Lemma 2 will show that, at a local minimum of the double well potential function, the Cauchy-Green strain can not be too small, at least no smaller than the negative of the second smallest material constant.

Lemma 1 *Assume that \underline{w} is a local minimizer of (6). It holds that*

$$\nabla g(\underline{w}) = \left(\left(\frac{1}{2}\|\underline{w}\|^2 - \nu \right) I + D \right) \underline{w} - \psi = 0, \quad (8)$$

$$\nabla^2 g(\underline{w}) = \underline{w} \underline{w}^T + \left(\frac{1}{2}\|\underline{w}\|^2 - \nu \right) I + D \succeq 0. \quad (9)$$

Lemma 2 Assume that $n \geq 2$ and \underline{w} is a local minimizer of (6). It holds that

$$\frac{1}{2}\|\underline{w}\|^2 - \nu + \alpha_2 \geq 0. \quad (10)$$

Furthermore, if $\alpha_1 < \alpha_2$, then

$$\frac{1}{2}\|\underline{w}\|^2 - \nu + \alpha_2 > 0. \quad (11)$$

Proof. Suppose that the statement (10) is false, then $\frac{1}{2}\|\underline{w}\|^2 - \nu + \alpha_2 < 0$. Hence $\frac{1}{2}\|\underline{w}\|^2 - \nu + \alpha_1 < 0$. Let $e_1^T = (1, 0, 0, \dots, 0)$ and $e_2^T = (0, 1, 0, \dots, 0)$. If $e_1^T \underline{w} = \underline{w}_1 = 0$, by the necessary condition (9), we have

$$0 \leq e_1^T (\underline{w} \underline{w}^T + (\frac{1}{2}\|\underline{w}\|^2 - \nu)I + D)e_1 = \frac{1}{2}\|\underline{w}\|^2 - \nu + \alpha_1 < 0, \quad (12)$$

which causes a contradiction. On the other hand, if $e_1^T \underline{w} \neq 0$, then, by (9) again, we have

$$\begin{aligned} 0 &\leq ((-\underline{w}_2)e_1 + (\underline{w}_1)e_2)^T (\underline{w} \underline{w}^T + (\frac{1}{2}\|\underline{w}\|^2 - \nu)I + D)((-\underline{w}_2)e_1 + (\underline{w}_1)e_2) \\ &= (\frac{1}{2}\|\underline{w}\|^2 - \nu + \alpha_1)(\underline{w}_2)^2 + (\frac{1}{2}\|\underline{w}\|^2 - \nu + \alpha_2)(\underline{w}_1)^2 < 0. \end{aligned}$$

It again causes a contradiction. Therefore, the statement (10) must be true.

When $\alpha_1 < \alpha_2$, suppose that the statement (11) is false, then we have

$$\frac{1}{2}\|\underline{w}\|^2 - \nu + \alpha_2 = 0. \quad (13)$$

By (13), we know that the second order necessary condition (9) becomes

$$0 \preceq \underline{w} \underline{w}^T + (\frac{1}{2}\|\underline{w}\|^2 - \nu)I + D = \underline{w} \underline{w}^T + D - \alpha_2 I. \quad (14)$$

Since the first two leading principal minors of the matrix in (14) are nonnegative, we have

$$\underline{w}_1^2 + \alpha_1 - \alpha_2 \geq 0 \quad (15)$$

and

$$\det \left\{ \begin{bmatrix} \underline{w}_1^2 & \underline{w}_1 \underline{w}_2 \\ \underline{w}_1 \underline{w}_2 & \underline{w}_2^2 \end{bmatrix} + \begin{bmatrix} \alpha_1 - \alpha_2 & 0 \\ 0 & 0 \end{bmatrix} \right\} = (\alpha_1 - \alpha_2) \underline{w}_2^2 \geq 0. \quad (16)$$

Remember that $\alpha_1 - \alpha_2 < 0$, inequality (15) implies that $\underline{w}_1 \neq 0$. Moreover, inequality (16) implies that $\underline{w}_2 = 0$. Together with (8), we obtain that $\psi_2 = 0$ and

$$\underline{w}_1 = \frac{2\psi_1}{\|\underline{w}\|^2 - 2\nu + 2\alpha_1} = \frac{-\psi_1}{\alpha_2 - \alpha_1}.$$

Without loss of generality, we assume that $\psi_1 < 0$, and hence $\underline{w}_1 > 0$. This implies, from (13) and the fact that $\underline{w}_2 = 0$, we have

$$\underline{w}_1 = \sqrt{2\nu - 2\alpha_2 - \sum_{i=3}^n \underline{w}_i^2}.$$

Consider the following parametric curve in \mathbb{R}^n :

$$\gamma(t) = \{(k(t), t, \underline{w}_3, \dots, \underline{w}_n) | k(t) = \sqrt{2\nu - 2\alpha_2 - t^2 - \sum_{i=3}^n \underline{w}_i^2} = \sqrt{\underline{w}_1^2 - t^2}, t \in R\} \quad (17)$$

where $\gamma(0) = \gamma(\underline{w}_2) = \underline{w}$, i.e., $\gamma(t)$ passes through \underline{w} at $t = 0$. Evaluating $g(w)$ on $\gamma(t)$, we have

$$\begin{aligned} g(\gamma(t)) &= \frac{1}{2} \left(\frac{k(t)^2}{2} + \frac{t^2}{2} + \frac{1}{2} \sum_{i=3}^n \underline{w}_i^2 - \nu + \alpha_1 \right)^2 - \alpha_1 \left(\frac{k(t)^2}{2} + \frac{t^2}{2} + \frac{1}{2} \sum_{i=3}^n \underline{w}_i^2 - \nu \right) - \frac{\alpha_1^2}{2} \\ &\quad + \frac{1}{2} \left(\alpha_1 k(t)^2 + \alpha_2 t^2 + \sum_{i=3}^n \alpha_i \underline{w}_i^2 \right) - \psi_1 k(t) - \sum_{i=3}^n \psi_i \underline{w}_i \\ &= \frac{(\alpha_2 - \alpha_1)^2}{2} + \frac{\alpha_2 - \alpha_1}{2} t^2 + \sum_{i=3}^n \frac{\alpha_i - \alpha_1}{2} \underline{w}_i^2 - \psi_1 \sqrt{\underline{w}_1^2 - t^2} - \sum_{i=3}^n \psi_i \underline{w}_i + \alpha_1 \alpha_2 - \frac{\alpha_1^2}{2}. \end{aligned}$$

It is not difficult to see that $t = 0$ is a local minimum point of $g(\gamma(w))$ since \underline{w} is a local minimizer of $g(w)$. However, this conclusion contradicts to the fact that

$$\frac{d}{dt}g(\gamma(0)) = \frac{d^2}{dt^2}g(\gamma(0)) = \frac{d^3}{dt^3}g(\gamma(0)) = 0; \quad \frac{d^4}{dt^4}g(\gamma(0)) = -\frac{3(\alpha_2 - \alpha_1)}{\underline{w}_1^2} < 0.$$

Therefore, the statement (11) must be true, if $\alpha_1 < \alpha_2$. \square

The next result Lemma shows that any critical point of the double well potential function having a sufficiently large Cauchy-Green strain (larger than the negative of all the material constants) must be a global minimum point.

Lemma 3 *Let w^* be a critical point of the function $g(w)$ in problem (6) with $\nabla g(w^*) = 0$. If*

$$\frac{1}{2} \|w^*\|^2 - \nu + \alpha_1 \geq 0, \quad (18)$$

then w^ is a global minimizer of problem (6). In particular, a local minimizer \underline{w} of problem (6) satisfying condition (18) must be a global minimizer.*

Proof. Define $Q = (\frac{1}{2} \|w^*\|^2 - \nu)I + D$. By the assumption that $\frac{1}{2} \|w^*\|^2 - \nu + \alpha_1 \geq 0$, it follows that

$\frac{1}{2}\|w^*\|^2 - \nu + \alpha_i \geq 0, \forall i \in [1 : n]$, and Q is positive semidefinite. Then,

$$\begin{aligned}
g(w) &= \frac{1}{2} \left(\frac{1}{2}\|w\|^2 - \nu \right)^2 + \frac{1}{2}w^T D w - \psi^T w \\
&= \frac{1}{2} \left(\frac{1}{2}\|w\|^2 - \nu \right)^2 - \frac{1}{2}w^T \left(\frac{1}{2}\|w^*\|^2 - \nu \right) I w + \frac{1}{2}w^T Q w - \psi^T w \\
&= \frac{1}{8}\|w\|^4 - \frac{1}{4}\|w\|^2\|w^*\|^2 + \frac{\nu^2}{2} + \frac{1}{2}w^T Q w - \psi^T w \\
&= \frac{1}{8}(\|w\|^2 - \|w^*\|^2)^2 + \frac{1}{2}w^T Q w - \psi^T w - \frac{1}{8}\|w^*\|^4 + \frac{\nu^2}{2} \tag{19}
\end{aligned}$$

$$\geq \frac{1}{2}w^T Q w - \psi^T w - \frac{1}{8}\|w^*\|^4 + \frac{\nu^2}{2} \tag{20}$$

$$\geq \frac{1}{2}w^{*T} Q w^* - \psi^T w^* - \frac{1}{8}\|w^*\|^4 + \frac{\nu^2}{2} \tag{21}$$

$$= g(w^*). \tag{22}$$

Since $Q \succeq 0$, the lower bound function expressed in (20) is a convex quadratic function. Its global minimum is attained at any \hat{w} satisfying $Q\hat{w} - \psi = (\frac{1}{2}\|w^*\|^2 - \nu)I\hat{w} + D\hat{w} - \psi = 0$. Since w^* is a critical point of (6), by equation (8) in Lemma 1, it is a global minimizer of the lower bound function in (20) and thus inequality (21) holds. Finally, (22) becomes true by substituting w^* into (19). \square

Theorem 1 *The double well potential problem (6) has at most one local, but non-global, minimizer.*

Proof. Let us assume that $n \geq 2$ first. Lemmas 2 and 3 imply that any local, but non-global, minimizer \underline{w} of problem (6) exists only if $\alpha_1 < \alpha_2$ and $-\alpha_2 < \frac{1}{2}\|\underline{w}\|^2 - \nu < -\alpha_1$. Consequently, we know the matrix $(\frac{1}{2}\|\underline{w}\|^2 - \nu)I + D$ is nonsingular with its first diagonal element being negative and others positive. Therefore, \underline{w} can be uniquely determined by equation (8) with

$$\underline{w}_i = \frac{2\psi_i}{\|\underline{w}\|^2 - 2\nu + 2\alpha_i}, \quad i \in [1 : n]. \tag{23}$$

From (9), we have $2\underline{w}_1^2 + \|\underline{w}\|^2 - 2\nu + 2\alpha_1 \geq 0$. Since $\|\underline{w}\|^2 - 2\nu + 2\alpha_1 < 0$, we know that

$$\underline{w}_1 \neq 0, \quad \psi_1 \neq 0 \quad \text{and} \quad 2\nu - 2\alpha_1 > \|\underline{w}\|^2 > 0. \tag{24}$$

Putting all \underline{w}_i together, we have

$$\sum_{i=1}^n \frac{4\psi_i^2}{(\|\underline{w}\|^2 - 2\nu + 2\alpha_i)^2} = \|\underline{w}\|^2.$$

In other words, the norm square of the local minimizer, i.e., $\|\underline{w}\|^2$, must be the root of the following secular function on a specific open interval:

$$h(t) = \sum_{i=1}^n \frac{4\psi_i^2}{(t - 2\nu + 2\alpha_i)^2} - t, \quad t \in (\max\{2\nu - 2\alpha_2, 0\}, 2\nu - 2\alpha_1). \tag{25}$$

Notice that each root of $h(t) = 0$ can only correspond to one local non-global minimizer of problem (6) using (23). Taking a simple calculation of (25), we have

$$h'(t) = -\sum_{i=1}^n \frac{8\psi_i^2}{(t - 2\nu + 2\alpha_i)^3} - 1, \quad (26)$$

$$h''(t) = \sum_{i=1}^n \frac{24\psi_i^2}{(t - 2\nu + 2\alpha_i)^4} > 0. \quad (27)$$

Therefore, the secular function $h(t)$ is a strictly convex function on $(\max\{2\nu - 2\alpha_2, 0\}, 2\nu - 2\alpha_1)$ with at most two roots. Furthermore, since $(\|\underline{w}\|^2 - 2\nu)I + 2D$ is nonsingular, the second order necessary condition (9) implies that

$$2(\Gamma\underline{w})(\Gamma\underline{w})^T + \text{Diag}(-1, 1, \dots, 1) \succeq 0,$$

where

$$\Gamma = \text{Diag} \left(\frac{1}{\sqrt{-\|\underline{w}\|^2 + 2\nu - 2\alpha_1}}, \frac{1}{\sqrt{\|\underline{w}\|^2 - 2\nu + 2\alpha_2}}, \dots, \frac{1}{\sqrt{\|\underline{w}\|^2 - 2\nu + 2\alpha_n}} \right). \quad (28)$$

Since its determinant is nonnegative, we have

$$0 \leq \det(2(\Gamma\underline{w})(\Gamma\underline{w})^T + \text{Diag}(-1, 1, \dots, 1)) \quad (29)$$

$$\begin{aligned} &= \det(\text{Diag}(-1, 1, \dots, 1)) \cdot \det(2\text{Diag}(-1, 1, \dots, 1)(\Gamma\underline{w})(\Gamma\underline{w})^T + I) \\ &= -1 \cdot (2(\Gamma\underline{w})^T \text{Diag}(-1, 1, \dots, 1)(\Gamma\underline{w}) + 1) \\ &= -\sum_{i=1}^n \frac{8\psi_i^2}{(\|\underline{w}\|^2 - 2\nu + 2\alpha_i)^3} - 1 \\ &= h'(t) \big|_{t=\|\underline{w}\|^2}. \end{aligned} \quad (30)$$

In other words, if \underline{w} is a local minimizer of problem (6), then it must satisfy the second order necessary condition (in matrix form) whose determinant is the first derivative of the secular function at $\|\underline{w}\|^2$. However, a strictly convex function has at most one root with a nonnegative first derivative. Thus we have shown the theorem for $n \geq 2$. When $n = 1$, it amounts to setting $\alpha_2 = \infty$ in the above analysis, and the proof follows. \square

The next corollary provides some simple sufficient conditions for having no local non-global minimizer.

Corollary 1 *When one of the following conditions is met:*

- (i) $2\nu - 2\alpha_1 \leq 0$ (in this case $g(w)$ is convex);
- (ii) $\alpha_1 = \alpha_2$;
- (iii) $\psi_1 = 0$;

(iv) $\max\{2\nu - 2\alpha_2, 0\} < 2\nu - 2\alpha_1$, $\psi_1 \neq 0$ and $\min_{t \in (\max\{2\nu - 2\alpha_2, 0\}, 2\nu - 2\alpha_1)} h(t) > 0$;

any local minimizer of the double well potential problem (6) is globally optimal.

Proof. (i) If $2\nu - 2\alpha_1 \leq 0$, then $\|w\|^2 - 2\nu + 2\alpha_i \geq 0$ for any $w \in R^n$ and $i \in [1 : n]$. Using the second derivative of $g(w)$ in (9), we have

$$\nabla^2 g(w) = 2ww^T + (\|w\|^2 - 2\nu)I + 2D \succeq 0,$$

which shows that $g(w)$ is indeed convex and any local optimum becomes globally optimal.

(ii) If \underline{w} is a local minimizer and $\alpha_1 = \alpha_2$, then inequality (10) in Lemma 2 and Lemma 3 imply that \underline{w} is indeed the global minimizer of problem (6).

(iii) If $\psi_1 = 0$, then equation (8) leads to either $\underline{w}_1 = 0$ or $\|\underline{w}\|^2 - 2\nu + 2\alpha_1 = 0$. By property (9), $\underline{w}_1 = 0$ further implies that $\|\underline{w}\|^2 - 2\nu + 2\alpha_1 \geq 0$. Using Lemma 3, both cases lead \underline{w} to be a global minimizer.

(iv) In this case, the secular function $h(t)$ actually does not have any solution in its domain. \square

The key result of establishing a necessary and sufficient condition for local, non-global minimizer is provided below.

Theorem 2 *The double well potential problem (6) has a local-nonglobal minimizer if and only if there is a $\underline{t}^* \in (\max\{2\nu - 2\alpha_2, 0\}, 2\nu - 2\alpha_1)$ such that the secular function $h(\underline{t}^*) = 0$ and $h'(\underline{t}^*) > 0$. Moreover, when it exists, the local non-global minimizer is given by*

$$\underline{w} = \left(\frac{2\psi_1}{\underline{t}^* - 2\nu + 2\alpha_1}, \dots, \frac{2\psi_n}{\underline{t}^* - 2\nu + 2\alpha_n} \right). \quad (31)$$

Proof. Suppose that $h(\underline{t}^*) = \sum_{i=1}^n \frac{4\psi_i^2}{(\underline{t}^* - 2\nu + 2\alpha_i)^2} - \underline{t}^* = 0$ with $\underline{t}^* \in (\max\{2\nu - 2\alpha_2, 0\}, 2\nu - 2\alpha_1)$. For the \underline{w} defined by (31), we have $\underline{t}^* = \|\underline{w}\|^2$ and \underline{w} satisfies the first order necessary condition (8). Moreover, the diagonal matrix $(\frac{1}{2}\|\underline{w}\|^2 - \nu)I + D$ is nonsingular with positive diagonal elements except for the first one. By Weyl's inequality (see [7], Theorem 4.3.1), we can estimate the largest $n - 1$ eigenvalues of the second order matrix $\underline{w}\underline{w}^T + (\frac{1}{2}\|\underline{w}\|^2 - \nu)I + D$ by

$$\begin{aligned} \sigma_i \left(\underline{w}\underline{w}^T + \left(\frac{1}{2}\|\underline{w}\|^2 - \nu \right) I + D \right) &\geq \sigma_1(\underline{w}\underline{w}^T) + \sigma_i \left(\left(\frac{1}{2}\|\underline{w}\|^2 - \nu \right) I + D \right) \\ &\geq \sigma_i \left(\left(\frac{1}{2}\|\underline{w}\|^2 - \nu \right) I + D \right) \\ &> 0, \quad \text{for } i = 2, 3, \dots, n. \end{aligned} \quad (32)$$

Since $h'(\underline{t}^*) > 0$, by (29) and (30), we have

$$\det \left(\underline{w}\underline{w}^T + \left(\frac{1}{2}\|\underline{w}\|^2 - \nu \right) I + D \right) = \frac{h'(\underline{t}^*)}{2\det^2(\Gamma)} > 0, \quad (33)$$

where Γ is defined in (28). Combining (32) with (33), we know that the smallest eigenvalue of the second order matrix must be positive, i.e., $\underline{w}\underline{w}^T + (\frac{1}{2}\|\underline{w}\|^2 - \nu)I + D \succ 0$. This is a sufficient condition to guarantee that \underline{w} is a local minimizer of problem (6).

On the hand side, let \underline{w} be a local, non-global minimizer of problem (6), which is unique quaranteed by Theorem 1. Let $\underline{t}^* = \|\underline{w}\|^2$. By the proof of Theorem 1, we know $\underline{t}^* \in (\max\{2\nu - 2\alpha_2, 0\}, 2\nu - 2\alpha_1)$. Moreover, \underline{w} can be expressed by \underline{t}^* as in (31) because \underline{w} satisfies the first order necessary condition (8). Also we have $h(\underline{t}^*) = 0$ and $h'(\underline{t}^*) \geq 0$. It remains for us to show that $h'(\underline{t}^*) > 0$. Suppose that, by contradiction, $h'(\underline{t}^*) = 0$. From (33), we have

$$\det \left(\underline{w}\underline{w}^T + (\frac{1}{2}\|\underline{w}\|^2 - \nu)I + D \right) = \frac{h'(\underline{t}^*)}{2\det^2(\Gamma)} = 0$$

and thus there is a $u = (u_1, \dots, u_n)^T \neq 0$ such that

$$\underline{w}\underline{w}^T u + \left((\frac{1}{2}\|\underline{w}\|^2 - \nu)I + D \right) u = 0. \quad (34)$$

From (34), we can write

$$u_i = \frac{-\underline{w}_i(u^T \underline{w})}{\frac{1}{2}\|\underline{w}\|^2 - \nu + \alpha_i}, \quad i = 1, 2, \dots, n.$$

Then, $u \neq 0$ implies that

$$u^T \underline{w} \neq 0. \quad (35)$$

Consider the double well potential function along the direction u defined by $q(\beta) := g(\underline{w} + \beta u)$. It is routine to verify that

$$\begin{aligned} q'(\beta) &= \nabla g(\underline{w} + \beta u)u, \\ q''(\beta) &= u^T \nabla^2 g(\underline{w} + \beta u)u, \\ q'''(\beta) &= 3u^T (\underline{w} + \beta u)u^T u. \end{aligned}$$

By the first order necessary condition (8), we have $q'(0) = 0$. By (9) and (34), we further have $q''(0) = 0$. However, (35) implies that

$$q'''(0) = 3(u^T \underline{w})(u^T u) \neq 0.$$

This result contradicts to the fact that \underline{w} is a local minimizer of problem (6). Therefore, $h'(\underline{t}^*) > 0$ and the proof is complete. \square

3 Characterization of global minimizer

In this section, we try to characterize different aspects of the global minimizer of the double well potential problem. We first observe that the double well potential function tends to $+\infty$ as $\|w\|^2 \rightarrow$

∞ . Therefore, the global minimizer of problem (6) always exists. Our first result is that each component of the global minimizer must be of the same sign as the corresponding component of the external force (i.e., the first-order term vector).

Lemma 4 *If w^* is the global minimizer of (6), then*

$$\psi_i w_i^* \geq 0, \quad i \in [1 : n]. \quad (36)$$

Proof. Let $\tilde{w} = (-w_1^*, w_2^*, w_3^*, \dots, w_n^*)$. Since the only odd-order term in $g(w)$ is the linear term, we have

$$g(w^*) - g(\tilde{w}) = -\psi_1(w_1^* - \tilde{w}_1) = -2\psi_1 w_1^* \leq 0.$$

Hence we know $\psi_1 w_1^* \geq 0$. A similar argument applies for any other components. \square

The next result shows that the sufficient condition $\frac{1}{2}\|w^*\|^2 - \nu + \alpha_1 \geq 0$ in Lemma 3 is indeed necessary for a critical point to become the global minimizer.

Theorem 3 *w^* is a global minimizer of (6) if and only if*

$$\nabla g(w^*) = \left(\left(\frac{1}{2}\|w^*\|^2 - \nu \right) + D \right) w^* - \psi = 0 \quad (37)$$

and

$$\|w^*\|^2 - 2\nu + 2\alpha_1 \geq 0. \quad (38)$$

Proof. The sufficiency is clear from Lemma 3. In addition, we can observe that the necessity of (37) follows immediately from equation (8). It remains to show that (38) is also a necessary condition.

To avoid triviality, we may assume that $\alpha_1 < \alpha_2$. Otherwise, by substituting $\alpha_1 = \alpha_2$ into (10), we can obtain the result at once. Suppose that $\|w^*\|^2 - 2\nu + 2\alpha_1 < 0$, then (9) implies that $2w_1^{*2} + \|w^*\|^2 - 2\nu + 2\alpha_1 \geq 0$. Hence we have $w_1^{*2} \neq 0$. Using (37), we have

$$2\psi_1 w_1^* = (\|w^*\|^2 - 2\nu + 2\alpha_1)w_1^{*2} < 0.$$

This causes a contradiction to Lemma 4 and the proof follows. \square

An immediate consequence of Theorem 3 is that the sign of the first component of the local non-global minimizer, if it exists, must be opposite to that of the first component of a global minimum solution.

Corollary 2 *If \underline{w} be the local non-global minimizer and w^* is a global minimizer of $g(w)$ of problem (6), then*

$$\text{sign}(\psi_1) = \text{sign}(w_1^*) = -\text{sign}(\underline{w}_1) \in \{-1, 1\}. \quad (39)$$

Proof. Since both \underline{w} and w^* are critical points, Theorem 3 implies that $\|\underline{w}\|^2 - 2\nu + 2\alpha_1 < 0$ and $\|w^*\|^2 - 2\nu + 2\alpha_1 \geq 0$. It follows from condition (iii) of Corollary 1 that $\psi_1 \neq 0$ and, from (8),

$$(\|\underline{w}\|^2 - 2\nu + 2\alpha_1)\underline{w}_1 = 2\psi_1, \quad (40)$$

$$(\|w^*\|^2 - 2\nu + 2\alpha_1)w_1^* = 2\psi_1. \quad (41)$$

Consequently, $\text{sign}(\underline{w}_1) = -\text{sign}(\psi_1) = -\text{sign}(w_1^*) \in \{-1, 1\}$. \square

In Section 4 of Part I, we have shown that the dual of the dual of the canonical primal problem (P) (see equation (19) of Part I) is equivalent to only a portion of (P) subject to n linear constraints (see equation (35) of Part I). Moreover, that portion contains the global minimizer. In the simplified version here, we have the third order term coefficient $\varphi = (\varphi_1, \varphi_2, \dots, \varphi_n)^T = 0$, which reduces the dual of the dual problem in Part I to the following problem:

$$\begin{aligned} P_0^{dd} = \inf_{\lambda \in \mathbb{R}^n} \quad & P^{dd}(\lambda) = \sum_{i=1}^n \alpha_i \lambda_i - \sum_{i=1}^n |\psi_i| \sqrt{2\lambda_i} + \frac{1}{2} \left(\sum_{i=1}^n \lambda_i - \nu \right)^2 \\ \text{s.t.} \quad & \lambda_i \geq 0, \quad i = 1, \dots, n. \end{aligned} \quad (42)$$

The portion of (P) corresponding to (42) becomes

$$\begin{aligned} \min_w \quad & \frac{1}{2} \left(\sum_{i=1}^n \frac{1}{2} w_i^2 - \nu \right)^2 + \sum_{i=1}^n \left\{ \frac{\alpha_i}{2} w_i^2 - \psi_i w_i \right\} \\ \text{s.t.} \quad & \psi_i w_i \geq 0, \quad i = 1, \dots, n \end{aligned} \quad (43)$$

under the nonlinear one-to-one map:

$$w_i = \begin{cases} \sqrt{2\lambda_i}, & \text{if } \psi_i \geq 0, \\ -\sqrt{2\lambda_i}, & \text{if } \psi_i < 0, \end{cases} \quad i = 1, \dots, n. \quad (44)$$

From Lemma 4, we know that the portion specified by (43) contains the global minimizer w^* . However, due to the opposite sign behavior on the first component, Corollary 2 implies that the local non-global minimizer \underline{w} is not in that portion. The mapping (44) was used to reveal the hidden convexity of (QP1QC) in Part I, but the local non-global minimizer is definitely excluded from the transformation. The missing of the local non-global minimizer can be seen clearly in Examples 1 and 2 of Part I.

4 Characterization of local maximizer

It is not difficult to see that the global maximum of problem (6) goes to $+\infty$ as $\|w\|^2$ grows without a bound. Hence there is no global maximizer of the problem. In this section, we provide an analytic study of the local maximizer of the simplified problem (6).

Lemma 5 *If \bar{w} is a local maximizer of (6), then*

$$\nabla g(\bar{w}) = \left(\frac{1}{2}\|\bar{w}\|^2 - \nu\right)\bar{w} + D\bar{w} - \psi = 0, \quad (45)$$

$$\nabla^2 g(\bar{w}) = \bar{w}\bar{w}^T + \left(\frac{1}{2}\|\bar{w}\|^2 - \nu\right)I + D \preceq 0. \quad (46)$$

The proof is easy. Moreover, it follows directly from (46) that

$$\frac{1}{2}\|\bar{w}\|^2 - \nu + \alpha_i \leq 0, \quad i = 1, 2, \dots, n. \quad (47)$$

In other words, at the local maximizer, the value of the Cauchy-Green strain is smaller than the negative value of all material constants.

Lemma 6 *If \bar{w} is a local maximizer of (6), then*

$$\psi_i = 0 \quad \text{if and only if} \quad \bar{w}_i = 0, \quad i = 1, 2, \dots, n.$$

Proof. It follows from (45) that

$$(\|\bar{w}\|^2 - 2\nu + 2\alpha_i)\bar{w}_i = \psi_i.$$

If $\bar{w}_i = 0$, then $\psi_i = 0$. On the other hand, if $\psi_i = 0$, it implies from $(\|\bar{w}\|^2 - 2\nu + 2\alpha_i)\bar{w}_i = 0$ that either $\|\bar{w}\|^2 - 2\nu + 2\alpha_i = 0$ or $\bar{w}_i = 0$ (or both). Suppose that $\|\bar{w}\|^2 - 2\nu + 2\alpha_i = 0$. It follows from (46) that

$$\bar{w}_i^2 + \frac{1}{2}\|\bar{w}\|^2 - \nu + \alpha_i = \bar{w}_i^2 \leq 0.$$

Therefore, \bar{w}_i must be also 0, and the proof follows. \square

Lemma 7 *If $\nu - \alpha_n \leq 0$, then the double well potential problem (6) has no local maximizer.*

Proof. If $\nu - \alpha_n < 0$, then (47) cannot be true and we have the conclusion. Now, assume that $\nu - \alpha_n = 0$. If (6) has a local maximizer \bar{w} , then it follows from (47) that $\|\bar{w}\| = 0$ or, equivalently, $\bar{w} = 0$. By Lemma 6, we have $\psi = 0$. It is routine to verify that

$$\begin{aligned} \frac{\partial g(w)}{\partial w_n} &= \left(\frac{1}{2}\|w\|^2 - \nu\right)w_n + \alpha_n w_n - \psi_n, \\ \frac{\partial^2 g(w)}{\partial^2 w_n} &= w_n^2 + \frac{1}{2}\|w\|^2 - \nu + \alpha_n, \\ \frac{\partial^3 g(w)}{\partial^3 w_n} &= 3w_n. \end{aligned}$$

Since $\bar{w} = 0$ and $\psi = 0$, we have

$$\frac{\partial g(\bar{w})}{\partial w_n} = \frac{\partial^2 g(\bar{w})}{\partial^2 w_n} = \frac{\partial^3 g(\bar{w})}{\partial^3 w_n} = 0. \quad (48)$$

Notice that

$$\frac{\partial^4 g(\bar{w})}{\partial^4 w_n} = 3 > 0.$$

Consequently, $\bar{w} = 0$ is not a local maximizer and we reached a contradiction. This completes the proof. \square

Lemma 8 *If $\nu - \alpha_n > 0$ and $\psi = 0$, then the double well potential problem (6) has a unique local maximizer $\bar{w} = 0$.*

Proof. Since $\nu - \alpha_n > 0$, $\psi = 0$ and $\alpha_1 \leq \dots \leq \alpha_n$, we have

$$\begin{aligned}\nabla g(0) &= 0, \\ \nabla^2 g(0) &= -\nu I + D \prec 0.\end{aligned}$$

Therefore, $\bar{w} = 0$ is a local maximizer of problem (6). Lemma 6 further guarantees that $\bar{w} = 0$ is the unique local maximizer. \square

Lemma 9 *If $\nu - \alpha_n > 0$ and $\psi \neq 0$, then the double well potential problem (6) has at most one local maximizer.*

Proof. Suppose \bar{w} is a local maximizer of (6). Since $\psi \neq 0$, we let $k \in [1 : n]$ be the largest nonzero index in $\{1, \dots, n\}$ such that

$$\psi_k \neq 0; \psi_{k+1} = \dots = \psi_n = 0. \quad (49)$$

In addition, let I_k be the identity matrix of order k and $D_k = \text{Diag}(\alpha_1, \dots, \alpha_k)$.

From equation (45), we have $(\|\bar{w}\|^2 - 2\nu + 2\alpha_k)\bar{w}_k = 2\psi_k$. Since $\psi_k \neq 0$, by Lemma 6, we know $\bar{w}_k \neq 0$, which implies that $\|\bar{w}\|^2 - 2\nu + 2\alpha_k \neq 0$. From inequality (47), we further know that $\|\bar{w}\|^2 - 2\nu + 2\alpha_k < 0$. Moreover, we have

$$\|\bar{w}\|^2 - 2\nu + 2\alpha_i < 0, \quad i = 1, \dots, k. \quad (50)$$

Consequently, matrix $(\|\bar{w}\|^2 - 2\nu)I_k + 2D_k$ is negative definite and, once $\|\bar{w}\|$ is computed, \bar{w}_i , $i = 1, 2, \dots, k$, can be uniquely determined by the following system of equations:

$$\bar{w}_i = \frac{2\psi_i}{\|\bar{w}\|^2 - 2\nu + 2\alpha_i}, \quad i = 1, \dots, k. \quad (51)$$

Since $\psi_{k+1} = \dots = \psi_n = 0$ implies that $\bar{w}_{k+1} = \dots = \bar{w}_n = 0$, it follows that any local maximizer \bar{w} must satisfy that

$$\sum_{i=1}^k \frac{4\psi_i^2}{(\|\bar{w}\|^2 - 2\nu + 2\alpha_i)^2} = \|\bar{w}\|^2.$$

From (27) and (50), we know $\|\bar{w}\|^2$ is a root of the following convex secular function:

$$h(t) = \sum_{i=1}^k \frac{4\psi_i^2}{(t - 2\nu + 2\alpha_i)^2} - t, \quad t \in [0, 2\nu - 2\alpha_k]. \quad (52)$$

Since matrix $(\|\bar{w}\|^2 - 2\nu)I_k + 2D_k$ is negative definite, from (46), we know that

$$-2(\Gamma_k \bar{w}^k)(\Gamma_k \bar{w}^k)^T + I_k \succeq 0,$$

where $\bar{w}^k = (\bar{w}_1, \dots, \bar{w}_k)^T$ and

$$\Gamma_k = \text{Diag} \left(\frac{1}{\sqrt{-\|\bar{w}\|^2 + 2\nu - 2\alpha_1}}, \dots, \frac{1}{\sqrt{-\|\bar{w}\|^2 + 2\nu - 2\alpha_k}} \right).$$

Then,

$$0 \leq \det(-2(\Gamma_k \bar{w}^k)(\Gamma_k \bar{w}^k)^T + I_k) \quad (53)$$

$$\begin{aligned} &= -2(\Gamma_k \bar{w}^k)^T (\Gamma_k \bar{w}^k) + 1 \\ &= \sum_{i=1}^k \frac{8\psi_i^2}{(\|\bar{w}\|^2 - 2\nu + \alpha_i)^3} + 1 \\ &= -h'(t) \big|_{t=\|\bar{w}\|^2} \cdot \text{(by (26))} \end{aligned} \quad (54)$$

Since a strictly convex function can have at most one root with its first derivative being non-positive, based on (51), we can conclude that there is at most one local maximizer. \square

Combining Lemmas 7, 8 and 9 together, we have the next result.

Theorem 4 *The double well potential problem (6) has at most one local maximizer.*

The above result can be further extended to obtain a necessary and sufficient condition under which a local maximum exists.

Theorem 5 *The double well potential problem (6) has a local maximizer if and only if $\nu - \alpha_n > 0$ and there is a $\bar{t}^* \in [0, 2\nu - 2\alpha_n)$ such that $h(\bar{t}^*) = 0$ and $h'(\bar{t}^*) < 0$ for the secular function defined in (52). Moreover, if it exists, the local maximizer \bar{w} is given by*

$$\bar{w} = \left(\frac{2\psi_1}{\bar{t}^* - 2\nu + 2\alpha_1}, \dots, \frac{2\psi_n}{\bar{t}^* - 2\nu + 2\alpha_n} \right). \quad (55)$$

Proof. (i) (if part) When $\psi = 0$, Lemma 8 assures that $\bar{w} = 0$ is the unique local maximizer of (6), which can be expressed as (55).

Now, consider $\psi \neq 0$. Let $k = 1, \dots, n$ be defined as in (49) and \bar{w} as in (55). Since $h(\bar{t}^*) = 0$ and $\bar{w}_{k+1} = \dots = \bar{w}_n = 0$, we have

$$\bar{t}^* = \sum_{i=1}^k \frac{4\psi_i^2}{(\bar{t}^* - 2\nu + 2\alpha_i)^2} = \|\bar{w}\|^2 \in [0, 2\nu - 2\alpha_n).$$

Then we see that \bar{w} satisfies the first order necessary condition (45). Moreover, we have

$$\left(\frac{1}{2}\|\bar{w}\|^2 - \nu\right)I + D \prec 0. \quad (56)$$

Let $\bar{w}^k = (\bar{w}_1, \dots, \bar{w}_k)^T$. Using Weyl's inequality (see [7], Theorem 4.3.1), we have

$$\begin{aligned} \sigma_i \left(\bar{w}^k (\bar{w}^k)^T + \left(\frac{1}{2}\|\bar{w}^k\|^2 - \nu\right)I_k + D_k \right) &\leq \sigma_i (\bar{w}^k (\bar{w}^k)^T) + \sigma_k \left(\left(\frac{1}{2}\|\bar{w}\|^2 - \nu\right)I_k + D_k \right) \\ &< \sigma_i (\bar{w}^k (\bar{w}^k)^T) \\ &= 0, \quad \text{for } i = 1, 2, \dots, k-1. \end{aligned}$$

Therefore, the first $k-1$ eigenvalues of the matrix $\bar{w}^k (\bar{w}^k)^T + (\frac{1}{2}\|\bar{w}\|^2 - \nu)I_k + D_k$ are negative. It follows from (53), (54) and the assumption of $h'(\bar{t}^*) < 0$ that

$$\det \left(-\bar{w}^k (\bar{w}^k)^T - \left(\frac{1}{2}\|\bar{w}\|^2 - \nu\right)I_k - D_k \right) = \frac{-h'(\bar{t}^*)}{2\det^2(\Gamma_k)} > 0. \quad (57)$$

If k is even, then

$$\det \left(\bar{w}^k (\bar{w}^k)^T + \left(\frac{1}{2}\|\bar{w}\|^2 - \nu\right)I_k + D_k \right) = \det \left(-\bar{w}^k (\bar{w}^k)^T - \left(\frac{1}{2}\|\bar{w}\|^2 - \nu\right)I_k - D_k \right) > 0,$$

which implies that the k^{th} eigenvalue of matrix $\bar{w}^k (\bar{w}^k)^T + (\frac{1}{2}\|\bar{w}\|^2 - \nu)I_k + D_k$ is negative.

If k is odd, then

$$\det \left(\bar{w}^k (\bar{w}^k)^T + \left(\frac{1}{2}\|\bar{w}\|^2 - \nu\right)I_k + D_k \right) = -\det \left(-\bar{w}^k (\bar{w}^k)^T - \left(\frac{1}{2}\|\bar{w}\|^2 - \nu\right)I_k - D_k \right) < 0,$$

which says that the k^{th} eigenvalue of matrix $\bar{w}^k (\bar{w}^k)^T + (\frac{1}{2}\|\bar{w}\|^2 - \nu)I_k + D_k$ is again negative. In other words, $\bar{w}^k (\bar{w}^k)^T + (\frac{1}{2}\|\bar{w}\|^2 - \nu)I_k + D_k \prec 0$. From (56), we have

$$\bar{w}\bar{w}^T + \left(\frac{1}{2}\|\bar{w}\|^2 - \nu\right)I + D = \begin{bmatrix} \bar{w}^k (\bar{w}^k)^T + \left(\frac{1}{2}\|\bar{w}\|^2 - \nu\right)I_k + D_k & 0 \\ 0 & \left(\frac{1}{2}\|\bar{w}\|^2 - \nu\right)I_{n-k} + D_{n-k} \end{bmatrix} \prec 0,$$

where $D_{n-k} = \text{Diag}(\alpha_{k+1}, \dots, \alpha_n)$. Consequently, \bar{w} satisfies the second order sufficient condition and becomes a local maximizer.

(ii) (only if part) Let \bar{w} be the unique local maximizer of (6). By Lemma 7, we have $\nu - \alpha_n > 0$. If $\psi = 0$, Lemma 8 implies that $\bar{w} = 0$. In this case, since $h(t) = -t$, there is a unique $\bar{t}^* = 0$ such that $h(\bar{t}^*) = 0$, $\bar{t}^* \in [0, 2\nu - 2\alpha_k)$ and $h'(\bar{t}^*) = -1 < 0$. The expression (55) follows immediately.

Assume that $\psi \neq 0$ with $\psi_k \neq 0$ and $\psi_{k+1} = \dots = \psi_n = 0$, and let $\bar{t}^* = \|\bar{w}\|^2$. From (52) and (54), we know $h(\bar{t}^*) = 0$, $\bar{t}^* \in [0, 2\nu - 2\alpha_k)$ and $h'(\bar{t}^*) \leq 0$. Then the expression for \bar{w} in (55) follows from (51) and $\bar{w}_{k+1} = \dots = \bar{w}_n = 0$. In the rest of the proof, we shall show a stronger result of which $\bar{t}^* \in [0, 2\nu - 2\alpha_n)$ and $h'(\bar{t}^*) < 0$.

First, if $k < n$, then $\psi_n = \bar{w}_n = 0$. From (47), we know $\bar{t}^* \in [0, 2\nu - 2\alpha_n]$. Suppose that $\bar{t}^* = 2\nu - 2\alpha_n$, similar to (48), we can verify that

$$\frac{\partial g(\bar{w})}{\partial w_n} = \frac{\partial^2 g(\bar{w})}{\partial^2 w_n} = \frac{\partial^3 g(\bar{w})}{\partial^3 w_n} = 0$$

and $\frac{\partial^4 g(\bar{w})}{\partial^4 w_n} = 3 > 0$. This is a contradiction to the fact that \bar{w} being a local maximizer of problem (6). Therefore, $\bar{t}^* \in [0, 2\nu - 2\alpha_n)$.

Next, we show that $h'(\bar{t}^*) < 0$. If not so, we consider $h'(\bar{t}^*) = 0$. By (57), we have

$$\det \left(-\bar{w}^k (\bar{w}^k)^T - \left(\frac{1}{2} \|\bar{w}\|^2 - \nu \right) I_k - D_k \right) = -h'(\bar{t}^*) / \det^2(\Gamma_k) = 0.$$

Consequently, matrix $\bar{w}^k (\bar{w}^k)^T + (\frac{1}{2} \|\bar{w}\|^2 - \nu) I_k + D_k$ is singular and there exists a $u = (u_1, \dots, u_k)^T \neq 0$ such that

$$\bar{w}^k (\bar{w}^k)^T u + \left(\left(\frac{1}{2} \|\bar{w}\|^2 - \nu \right) I_k + D_k \right) u = 0. \quad (58)$$

Equivalently,

$$u_i = \frac{-\bar{w}_i (u^T \bar{w}^k)}{\frac{1}{2} \|\bar{w}\|^2 - \nu + \alpha_i}, \quad i = 1, 2, \dots, k.$$

Since $u \neq 0$, we know $u^T \bar{w}^k \neq 0$. Define

$$\tilde{u} = (u_1, \dots, u_k, 0, \dots, 0)^T \in R^n.$$

Then, we have

$$\tilde{u}^T \tilde{u} \neq 0, \quad \tilde{u}^T \bar{w} = u^T \bar{w}^k \neq 0. \quad (59)$$

Similar to the proof of Theorem 2, we can consider $q(\beta) := g(\bar{w} + \beta \tilde{u})$. It follows that

$$\begin{aligned} q'(\beta) &= \nabla g(\bar{w} + \beta \tilde{u}) \tilde{u}, \\ q''(\beta) &= \tilde{u}^T \nabla^2 g(\bar{w} + \beta \tilde{u}) \tilde{u}, \\ q'''(\beta) &= 3 \tilde{u}^T (\bar{w} + \beta \tilde{u}) \tilde{u}^T \tilde{u}. \end{aligned}$$

Since \bar{w} satisfies the first order necessary condition (45), $q'(0) = 0$. By (58), we have $q''(0) = 0$. Moreover, (59) implies that $q'''(0) = 3(\tilde{u}^T \bar{w})(\tilde{u}^T \tilde{u}) \neq 0$. Consequently, 0 is not a local maximizer of $q(\beta)$ and \bar{w} is not a local maximizer, which causes a contradiction. Therefore, we know $h'(\bar{t}^*) < 0$. This completes the proof. \square

The next result shows that, when it exists, the unique local maximizer is “surrounded” by all local (non-global and global) minimizers.

Theorem 6 *If \underline{w} is a local minimizer and \bar{w} is the local maximizer of the double well potential problem (6), then*

$$\|\bar{w}\| < \|\underline{w}\|. \quad (60)$$

Proof. (i) $n \geq 2$: If $\alpha_1 < \alpha_2$, following Lemma 2 and (47), we have

$$\|\underline{w}\|^2 > 2\nu - 2\alpha_2 \geq \|\overline{w}\|^2.$$

Otherwise, $\alpha_1 = \alpha_2$ and we assume that $\|\overline{w}\| = \|\underline{w}\|$. Applying Lemma 2 and (47) again, we have

$$\|\underline{w}\|^2 = 2\nu - 2\alpha_1 = 2\nu - 2\alpha_2 = \|\overline{w}\|^2.$$

Since both \underline{w} and \overline{w} are critical points of $g(w)$, Lemma 3 implies that both of them are global minimizers, which is impossible. Therefore, $\|\overline{w}\| < \|\underline{w}\|$.

(ii) $n = 1$: If $\psi_1 = 0$, then the first order necessary condition (45) implies that either $\overline{w} = 0$ or $\overline{w}^2 - 2\nu + 2\alpha_1 = 0$. Since \overline{w} can not be a global minimizer, the latter case is eliminated and thus $\overline{w} = 0$. To prove (60), it is sufficient to show that $\underline{w} \neq 0$. Suppose that $\underline{w} = 0$, then the second order necessary condition (9) implies that

$$0 \leq 2\underline{w}^2 + \underline{w}^2 - 2\nu + 2\alpha_1 = -2\nu + 2\alpha_1. \quad (61)$$

By Corollary 1 (i), $g(w)$ is convex and hence the local maximizer \overline{w} does not exist, which causes a contradiction to the setting of the theorem.

If $\psi_1 \neq 0$, then $w^2 - 2\nu + 2\alpha_1 \neq 0$ for any local minimizer or maximizer w . Therefore, $t_1 = \underline{w}^2$ and $t_2 = \overline{w}^2$ are two solutions to the following equation:

$$h(t) = \frac{4\psi_1^2}{(t - 2\nu + 2\alpha_1)^2} - t = 0,$$

From the proofs of Theorem 1 and Theorem 4, we have

$$\begin{aligned} h'(t) \big|_{t=\underline{w}^2} &\geq 0, \\ h'(t) \big|_{t=\overline{w}^2} &\leq 0. \end{aligned}$$

Since $h(t)$ is strictly convex, it has two distinct solutions satisfying the above first order conditions only when $\underline{w}^2 > \overline{w}^2$. This completes the proof. \square

5 Computational algorithms

According to Corollaries 2 and 5, the local, non-global minimizer and the local maximizer of the simplified version of (6), if they exist, are closely related to the convex secular function $h(t)$ over different intervals. The convex secular function $h(t)$ is a convenient substitute for the first order necessary condition, while the intervals capturing the root of $h(t)$ reflect the second order necessary condition. The sign of the first derivative of $h(t)$ at the root provides necessary and sufficient conditions for the type of a local extremum, namely, positive sign for the local, but non-global, minimizer; negative sign for the local maximizer.

The necessary and sufficient condition for the global minimum w^* in Theorem 3 can also be expressed in terms of the secular function $h(t)$. From (38), we have $\|w^*\|^2 \in [2\nu - 2\alpha_1, \infty)$. If $\|w^*\|^2 > 2\nu - 2\alpha_1$, (37) implies that $h(\|w^*\|^2) = 0$. Moreover, by (26),

$$h'(\|w\|^2) = - \sum_{i=1}^n \frac{8\psi_i^2}{(\|w\|^2 - 2\nu + 2\alpha_i)^3} - 1 < 0 \text{ for } \|w\|^2 > 2\nu - 2\alpha_1.$$

It implies that $h(t)$ is monotonically decreasing on $(2\nu - 2\alpha_1, \infty)$ and the unique root $\|w^*\|^2$ must recover w^* .

Otherwise, if $\|w^*\|^2 = 2\nu - 2\alpha_1$, the secular function $h(t)$ is singular at $\|w^*\|^2$ and there could be multiple global minimum solutions. In this case, let \bar{k} be the index such that $\alpha_1 = \alpha_2 = \dots = \alpha_{\bar{k}} < \alpha_{\bar{k}+1}$. The first order necessary condition $(\frac{1}{2}\|w\|^2 - \nu + D)w = \psi$ can be solved by letting $w = (-\alpha_1 I + D)^+ \psi + \sum_{i=1}^{\bar{k}} \gamma_i e_i$, where $(\cdot)^+$ denotes the Moore-Penrose generalized inverse; γ_i are free parameters and e_i is the i -th column of I . Then, we can establish the following *generalized secular equation*

$$\|w\|^2 = \|(-\alpha_1 I + D)^+ \psi + \sum_{i=1}^{\bar{k}} \gamma_i e_i\|^2 = 2\nu - 2\alpha_1 \quad (62)$$

from which we try to find solution(s) $\gamma = \gamma^* = (\gamma_1^*, \dots, \gamma_{\bar{k}}^*)$. Since the vector $(-\alpha_1 I + D)^+ \psi$ is perpendicular to each vector of $\gamma_i^* e_i$, we have

$$\sum_{i=1}^{\bar{k}} \gamma_i^{*2} = 2\nu - 2\alpha_1 - \|(-\alpha_1 I + D)^+ \psi\|^2. \quad (63)$$

If $\bar{k} = 1$ and $2\nu - 2\alpha_1 - \|(-\alpha_1 I + D)^+ \psi\|^2 > 0$, there are exactly two global optimal solutions. If $\bar{k} \geq 2$ and $2\nu - 2\alpha_1 - \|(-\alpha_1 I + D)^+ \psi\|^2 > 0$, there are infinitely many global solutions which form a k -dimensional sphere. The result coincides with Theorem 1 of Part I. If $2\nu - 2\alpha_1 - \|(-\alpha_1 I + D)^+ \psi\|^2 = 0$, the optimal solution set degenerates to a singleton $w^* = (-\alpha_1 I + D)^+ \psi$.

In summary, we provide three algorithms for finding the global minimizers, local non-global minimizer and local maximizer, respectively.

Algorithm 1 (*finding global minimizers*)

Step 1: Solve the equation of one variable

$$h(t) = \|[(\frac{1}{2}t - \nu)I + D]^{-1}\psi\|^2 - t = 0, \quad t \in (2\nu - 2\alpha_1, \infty).$$

If there is a solution t^ , Stop! The unique global minimizer of the double well potential problem (6) is*

$$w^* = [(\frac{1}{2}t^* - \nu)I + D]^{-1}\psi.$$

Otherwise, go to Step 2.

Step 2 If $\alpha_1 < \alpha_2$ and $\bar{k}=1$, solve equation (63) for at most two solutions:

$$\gamma_1^* = \pm \sqrt{2\nu - 2\alpha_1 - \|(-\alpha_1 I + D)^+ \psi\|^2}.$$

If $\gamma_1^* \neq 0$, the double well potential problem (6) has exactly two global minimizers of the form

$$w^* = (-\alpha_1 I + D)^+ \psi + \gamma_1^* e_1.$$

If $\gamma_1^* = 0$, $w^* = (-\alpha_1 I + D)^+ \psi$ is the unique global minimizer.

Step 3 If $\bar{k} \geq 2$, the double well potential problem (6) has one or infinitely many global minimizers:

$$w_i^* = (-\alpha_1 I + D)^+ \psi + \sum_{i=1}^{\bar{k}} \gamma_i^* e_i,$$

where $(\gamma_1^*, \dots, \gamma_{\bar{k}}^*)$ are obtained by solving (63).

If $\sqrt{2\nu - 2\alpha_1 - \|(-\alpha_1 I + D)^+ \psi\|^2} = 0$, $w^* = (-\alpha_1 I + D)^+ \psi$ is the unique optimal solution.

Otherwise, the global optimal solutions form a sphere centered at $(-\alpha_1 I + D)^+ \psi$ with the radius of $\sqrt{2\nu - 2\alpha_1 - \|(-\alpha_1 I + D)^+ \psi\|^2}$.

Algorithm 2 (finding local non-global minimizer)

Solve the equation

$$h(t) = \|[(\frac{1}{2}t - \nu)I + D]^{-1} \psi\|^2 - t = 0, \quad t \in (\max\{2\nu - 2\alpha_2, 0\}, 2\nu - 2\alpha_1).$$

If there is a solution \underline{t}^* such that $h'(\underline{t}^*) > 0$, the unique local non-global minimizer of the double well potential problem (6) is

$$\underline{w} = [(\frac{1}{2}\underline{t}^* - \nu)I + D]^{-1} \psi.$$

Otherwise, declare that there is no local non-global minimizer.

Algorithm 3 (finding the local maximizer)

Step 1 If $\nu - \alpha_n \leq 0$, declare that there is no local maximizer.

If $\nu - \alpha_n > 0$ and $\psi = 0$, then 0 is the unique local maximizer.

Otherwise, go to Step 2.

Step 2 Solve the equation

$$h_+(t) = \|[(\frac{1}{2}t - \nu)I + D]^+\psi\|^2 - t = 0, \quad t \in [0, 2\nu - 2\alpha_n).$$

If there is a solution \bar{t}^* such that $h'(\bar{t}^*) < 0$, then the unique local maximizer of the double well potential problem (6) is

$$\bar{w}^* = [(\frac{1}{2}\bar{t}^* - \nu)I + D]^+\psi.$$

Otherwise, declare that there is no local maximizer.

Notice that each of the above three algorithms can be done in a polynomial time since the main computation involved is to solve the secular equation in one variable. To illustrate their numerically behavior, we use the same data set of (A, B, c, d, f) of the three examples in Part I of this paper and apply the space reduction in Section 2 to convert the testing problems into the format of (6).

Example 1 (Example 1 of Part I:) Let $n = 1$ and $\nu = 14$, $\alpha_1 = -2$, $\psi_1 = -3$, the double well potential problem becomes

$$\min \left\{ g(w) = \frac{1}{2} \left(\frac{1}{2}w^2 - 14 \right)^2 - w^2 + 3w \right\}.$$

The corresponding function $g(w)$ is shown in Figure 2.

In this example, there are one global minimizer, one local non-global minimizer and one local maximizer. The secular function

$$h(t) = \frac{36}{(t - 32)^2} - t \tag{64}$$

is shown in Figure 2. By finding the root of (64) in $(2\nu - 2\alpha_1, \infty) = (32, \infty)$, Algorithm 1 provides a solution $t^* = 33.0438$ and we find the global minimizer $w^* = -5.7484$ with the value of -47.1089 . For the local non-global minimizer, we apply Algorithm 2 to find the root of (64) in $(\max\{2\nu - 2\alpha_2, 0\}, 2\nu - 2\alpha_1) = (0, 32)$. Algorithm 2 returned $\underline{t}^* = 30.9210$ with $h'(\underline{t}^*) = 56.3138 > 0$, which concluded that the local non-global minimizer is $\underline{w}^* = 5.5607$ with the value of -13.1725 . As for the local maximizer, by finding the root of (64) in $[0, 2\nu - 2\alpha_n) = [0, 32)$, Algorithm 3 returned $\bar{t}^* = 0.0352$ with $h'(\bar{t}^*) = -0.9978 < 0$. It led to the local maximizer $\bar{w}^* = 0.1877$ with the value of 98.2814 .

Notice that the signs of the two minimizers, $w^* = -5.7484$ and $\underline{w}^* = 5.5607$, are different, which demonstrates Corollary 2. The numerical results also showed that the local maximizer $\bar{w}^* = 0.1877$ locates between the two minimizers, which is claimed by Theorem 6.

Example 2 (Example 2 of Part I:) Applying the space reduction technique, we obtain the double well potential problem in the format of (6) with the data $n = 2$ and

$$\nu = 27.9994, \quad D = \begin{bmatrix} -1.9960 & 0 \\ 0 & 202.0700 \end{bmatrix}, \quad \psi = \begin{bmatrix} -22.0487 \\ -502.0209 \end{bmatrix}.$$

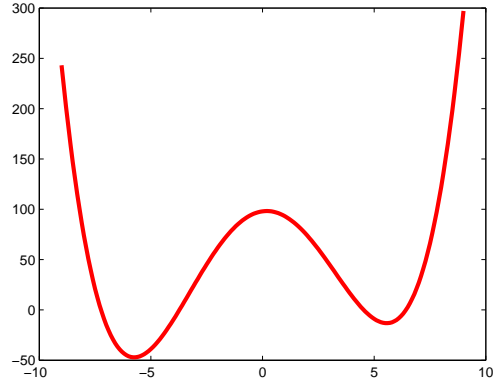


Figure 2: The graph of $g(w)$ in Example 1 ($n = 1$).

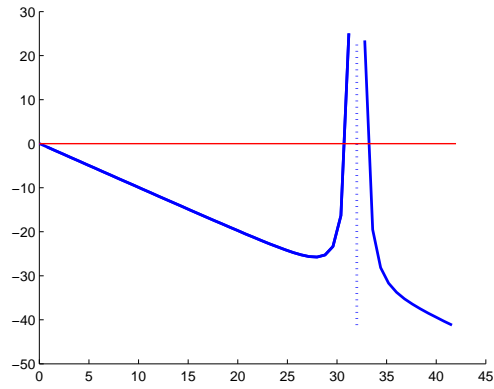


Figure 3: The secular function (64).

The corresponding function $g(w)$ and its contour are shown in Figure 4.

Its secular function becomes

$$h(t) = \frac{1944.5808}{(t - 59.9908)^2} + \frac{1008099.9361}{(t + 350.14)^2} - t \quad (65)$$

(shown in Figure 5). Finding the root of (65) on $(2\nu - 2\alpha_1, \infty) = (59.9908, \infty)$ results in $t^* = 65.6930$, Algorithm 1 gives the global minimizer $w^* = \begin{bmatrix} -7.7335 \\ -2.4262 \end{bmatrix}$ with the value of -841.7182 . Similarly, finding the root of (65) in $(\max\{2\nu - 2\alpha_2, 0\}, 2\nu - 2\alpha_1) = (0, 59.9908)$ results in $\underline{t}^* = 53.5813$. Since $h'(\underline{t}^*) = 13.7390 > 0$, Algorithm 2 provides the local non-global minimizer $\underline{w}^* = \begin{bmatrix} 6.8800 \\ -2.4993 \end{bmatrix}$ with the value of -518.3996 . Notice that the signs of the first component of the two minimizers are different, which demonstrates Corollary 2. Finally, since $2\nu - 2\alpha_n = -348.1412 < 0$, Algorithm 3 says that there is no local maximizer for this example.

Example 3 (*Maxican Hat Example*) In this example,

$$g(w) = \frac{1}{2}(\frac{1}{2}w_1^2 + \frac{1}{2}w_2^2 - 38)^2,$$

which is already in the format of (6) with $n = 2$,

$$\nu = 38, \quad D = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}, \quad \psi = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

The graph of the Maxican hat function $g(w)$ and its contour are shown in Figure 6.

Since $\alpha_1 = \alpha_2 = 0$ and $2\nu - 2\alpha_1 = 76$, the secular function

$$h(t) = -t, \quad t \neq 76 \quad (66)$$

has a unique solution 0 and it becomes singular at $t = 76$. Algorithm 1 stopped at Step 3 and claimed that

$$w^* = \{(\gamma_1^*, \gamma_2^*) \mid (\gamma_1^*)^2 + (\gamma_2^*)^2 = 76\}.$$

is the set of global optimal solutions with the optimal value of 0.

Since $(\max\{2\nu - 2\alpha_2, 0\}, 2\nu - 2\alpha_1) = (76, 76) = \emptyset$, Algorithm 2 returned an answer that there is no local non-global minimizer. It is clear that (66) has a unique root $\bar{t}^* = 0$ on $[0, 2\nu - 2\alpha_n) = [0, 76)$ and $h'(\bar{t}^*) = -1 < 0$. Since $\psi = 0$, Algorithm 3 returned the unique local maximizer $\bar{w}^* = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$.

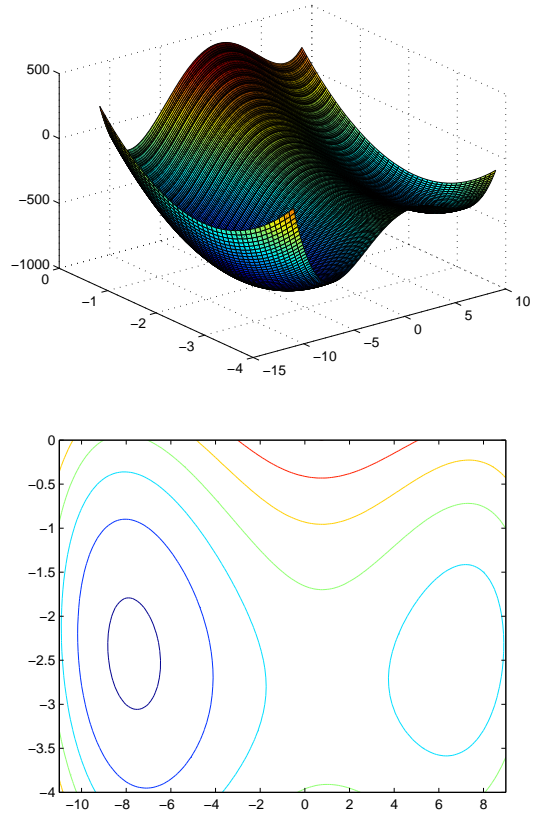


Figure 4: The function $g(w)$ in Example 2 and its contour ($n = 2$).

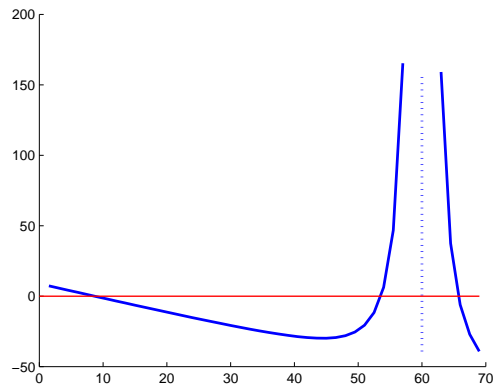


Figure 5: The secular function (65).

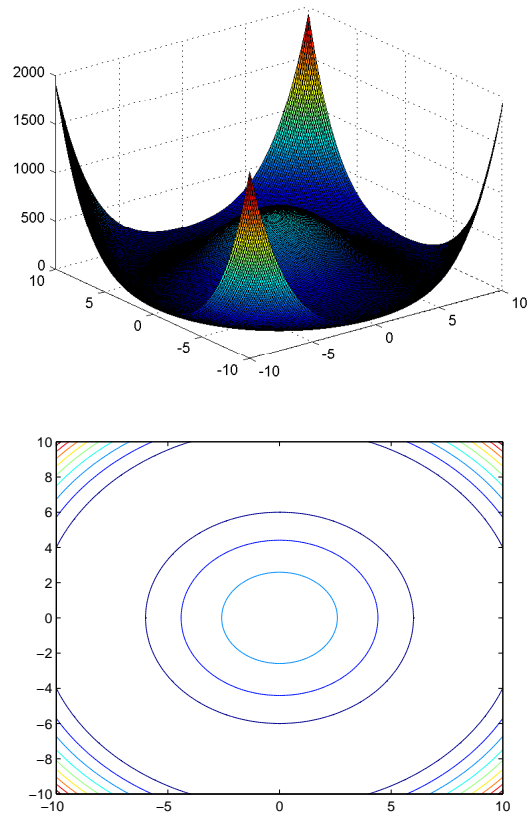


Figure 6: The function $g(w)$ in Example 3 and its contour ($n = 2$).

6 Conclusions

In this paper we have characterized the local minimizers and maximizers of the double well potential problem. By analyzing the first and the second order necessary conditions and through the study of the corresponding secular functions, we are able to estimate the number of local optimizers and locate each of them. Moreover, the convex secular functions (equations) are used to characterize sufficient and necessary conditions for all types of optimizers with explicit computational algorithms developed for finding them. The (DWP) problem is a special case of the more general quadratic programming problem with one quadratic constraint (QP1QC). We expect that the analytical techniques developed in this paper can be extended to study (QP1QC) and other quadratic programming problems.

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